Sebacic acid, 1-(4-fluorophenyl)ethyl pentyl ester

Inchi: InChI=1S/C23H35FO4/c1-3-4-11-18-27-22(25)12-9-7-5-6-8-10-13-23(26)28-19(2)20-14-1

InchiKey: SGKHOWHITQVVOT-UHFFFAOYSA-N

Formula: C23H35FO4

SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OC(C)c1ccc(F)cc1

Mol. weight [g/mol]: 394.52

Physical Properties

Property code	Value	Unit	Source
gf	-419.53	kJ/mol	Joback Method
hf	-983.98	kJ/mol	Joback Method
hfus	54.11	kJ/mol	Joback Method
hvap	86.84	kJ/mol	Joback Method
log10ws	-7.07		Crippen Method
logp	6.284		Crippen Method
mcvol	327.820	ml/mol	McGowan Method
pc	1071.46	kPa	Joback Method
rinpol	2658.00		NIST Webbook
rinpol	2658.00		NIST Webbook
tb	908.71	K	Joback Method
tc	1113.66	K	Joback Method
tf	517.82	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1065.62	J/mol×K	908.71	Joback Method
cpg	1082.18	J/mol×K	942.87	Joback Method
cpg	1097.44	J/mol×K	977.03	Joback Method
cpg	1111.45	J/mol×K	1011.19	Joback Method
cpg	1124.23	J/mol×K	1045.35	Joback Method
cpg	1135.82	J/mol×K	1079.50	Joback Method
cpg	1146.25	J/mol×K	1113.66	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380739&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume